Weakening of antiferromagnetism due to frustration on inhomogeneous 2D lattices

Anuradha Jagannathan
Laboratoire de Physique des Solides, Université Paris-Sud, 91405 Orsay, France
E-mail: jagannathan@lps.u-psud.fr

Abstract. I consider the ground state of quantum spins interacting via Heisenberg antiferromagnetic exchange, in lattices having several types of local environment. In unfrustrated cases, when a Néel type order exists, it is known that quantum fluctuations are site-dependent, and lead to an inhomogeneous local staggered order parameter. This paper discusses some effects of adding frustration to such a system, by including next nearest neighbor antiferromagnetic interactions. Within linear spinwave theory, it is found that as the frustration parameter increases, the local order parameters decrease at a rate that depends on the type of sites involved in the frustrated loops. The cases of a decorated square lattice system, and of a quasiperiodic tiling are considered to study different ways in which antiferromagnetism is suppressed in these inhomogeneous systems.

1. Introduction

The work reported here is a study of the different means of suppressing antiferromagnetic order by frustration, in systems with several local environments for spins. The calculations are carried out within spin wave theory. Their starting point is the Néel ordered ground state of $S = \frac{1}{2}$ Heisenberg models in unfrustrated two dimensional (2D) lattices in which all couplings are short-range, antiferromagnetic and of equal magnitude, denoted by J. The structures I consider are inhomogeneous in that their unit cell contains sites having different coordination numbers. The classical antiferromagnetic ground state for such systems has a collinear two-sublattice Néel ordering with a staggered local magnetization $m_{si} = \epsilon_i \langle S_i^z \rangle = \frac{1}{2}$ uniformly on all sites, where $\epsilon_i = \pm 1$ depending on whether the site i belongs to the A(B) sublattice, and z is the axis of symmetry breaking. The quantum ground state is inhomogeneous [1], with varying m_{si} values. The staggered moment tends to be large, for example, on sites with smallest coordination number z (not to be confused with the spatial z-direction) [2].

When additional frustrating interactions are added to the original Heisenberg Hamiltonian via J' exchange terms that antiferromagnetically couple spins belonging to the same sublattice, both the global staggered moment, as well as the local order parameters will eventually be suppressed for large enough J', when the system goes over to a new state: a coplanar state, or nonmagnetic spin liquid state, for example. Spin wave theory, which works well for small J' will also break down before the transition occurs. Results will be presented for a range of values $0 < J' < J'_u$, where J'_u is the value of the exchange interaction J' for which linear spin wave theory becomes unstable.

I discuss first a simple square lattice ferrimagnetic example, in which the sublattices are of unequal size (i.e. the number of sites in the A-sublattice, N_A is half that of the B-sublattice

$N_B = 2N_A$) to illustrate this effect. I will then consider a more complicated example of a quasiperiodic case with two equal sublattices, which has an $S = 0$ collinear Néel type ground state.

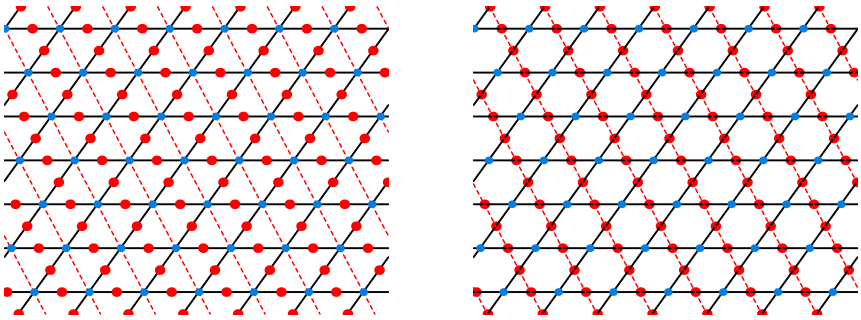

Figure 1. Decorated square lattice system showing the J bonds (blue) and J' bonds (dashed red) for cases I (left) and II(right). Sites of the A(B) sublattice spins are shown in blue (red).

2. The decorated square lattice

The unperturbed Heisenberg Hamiltonian is

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i . \vec{S}_j \tag{1}$$

where the spins are placed on the vertices of the square lattice (the A-sublattice), and on midpoints of each of the sides of the squares (the B-sublattice). The exchange interaction J, represented in blue in Figs.1, gives rise to a staggered arrangement of spin up on the A-sublattice and spin down on the B-sublattice. Since the number of sites in the two sublattices is unequal, there will be a net magnetization, and this is reflected in the magnon spectrum. Low energy modes have energy increasing as the square of the wave number, $\omega(k) \sim k^2$ instead of linearly in k, as for the example that will be discussed next.

In linear spin wave theory, the quantum corrections for the onsite staggered magnetization (see [1] for a description of similar models) gives $m_s^{(A)} \approx 0.28$ and $m_s^{(B)} \approx 0.38$ for the two sublattices. The large difference of values of sublattice magnetization in this (and similar models) is in keeping with results of Quantum Monte Carlo simulations. The difference can be explained by an argument based on the Heisenberg star cluster [1] – consisting of a central spin connected to z nearest neighbors – for which the quantum fluctuations about a Néel ordered state are z-fold stronger for the center spin compared to the spins on the extremities. This qualitatively explains the smaller staggered moment on the A-sublattice sites (coordination number $z = 4$) compared to the B-sublattice sites (for which $z = 2$).

We now consider two different ways of introducing frustration, which are illustrated in Figs.1a and b). In case I, bonds are added along the diagonals of the square lattice: the A-sublattice spins are coupled via a new term $J'\vec{S}_i.\vec{S}_j$. For small enough J', such that the symmetry of the ground state is not changed, this leads to a change in the classical ground state energy per site of $\Delta E_0/N = J'S^2/3$. Note: in the figures, bond angles and distances have been distorted, to emphasize the relation to the triangular lattice system, but not the topological connectivity, which remains that of the square lattice system when $J' = 0$.

In case II, the new terms link spins lying on the B-sublattice, $(i, j \in B)$. The change in ground state energy per site in this case is given by $\Delta E_0/N = 2J'S^2/3$. The parameter $f = \Delta E_0/NS^2$ will be used below as a measure of the frustration in each of the two cases considered.

Although our calculations are valid for a large range of J', we note that our concept of slightly perturbing the original topology is only valid for small J'. As J' becomes large, case II, for example, is better considered as an anisotropic Kagome system, since all sites have the same connectivity.

2.1. Case I. Frustration via coupling between high z lattice sites
As J' increases, the staggered magnetization decreases on both sublattices, as one can see from the red (sublattice A) and blue (sublattice B) curves in Fig.2 which are marked Case I. The f parameter is given by $f = J'/3$ for these two curves, which extend out to a value of f determined by the point at which linear spin wave theory around the collinear state becomes unstable.

2.2. Case II. Frustration via coupling between low z lattice sites
As J' increases, the staggered magnetization decreases on both sublattices, as one can see from the red (sublattice A) and blue (sublattice B) curves in Fig.2 which are marked Case II. The f parameter is defined by $f = 2J'/3$ for these two curves. Linear spin wave theory becomes unstable in this case for a value of $f \approx 0.33$. As can be seen in the figure, the changes in the staggered order parameters as a function of f are relatively smaller in this case.

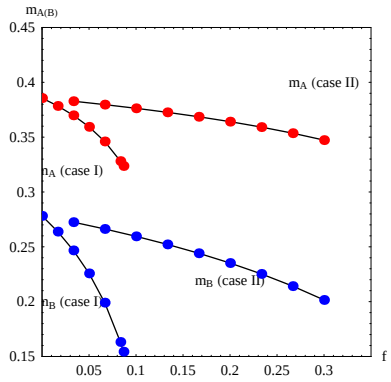

Figure 2. Plot of staggered magnetization for the A and B sublattice sites for cases I and II

This example shows the influence of the local environment: frustration effects can be greater or smaller depending on the type of sites linked by the J' terms. In this example, as J' is "turned on", one finds a larger suppression of the global and local order parameters for the situation where the high-z sites are involved. For these sites, the big quantum fluctuations induced by large nearest neighbor number are enhanced by the frustrating terms. The next example considers frustration in a more complex model in which A- and B-sublattices are equivalent, and each one has many different local environments.

3. Penrose tiling antiferromagnet

The Penrose rhombus tiling, considered here, is bipartite with two equivalent sublattices. Numerical calculations of the spin wave spectrum were carried out for finite systems with $N_A = N_B$, which possess an $S = 0$ ground state, for the unperturbed $J' = 0$ Hamiltonian. The figures 3 show the strong J bonds in blue. These bonds act along the tile edges of the two building blocks of the Penrose tiling, the 36° – or thin – rhombus and the 72° – or thick – rhombus). The new frustration-inducing diagonal J' bonds are shown in red for two different situations. Case III corresponds to connecting sites across the diagonal of the thick rhombuses,

while case IV corresponds to connecting sites on the diagonals of the thin rhombuses. Note that these bonds connect different classes of sites, and affect A- and B-sublattices equally. The J' bonds frustrate sites to different degrees, the classification of sites into families depending largely on their coordination number, which ranges from 3 to 7. An inspection of the figures will make it clear that, for example, the connectivities of $z = 6$ and $z = 7$ vertices are not modified. In brief, the J' terms have their strongest effects on a subset of $z = 5$ sites for the case III and $z = 4$ sites in case IV.

The frustration parameter f, determined by the shift in the classical ground state energy as in the previous square lattice example, here takes the values $f = 0.56J'$ (case III) and $f = 0.38J'$ (case IV) respectively.

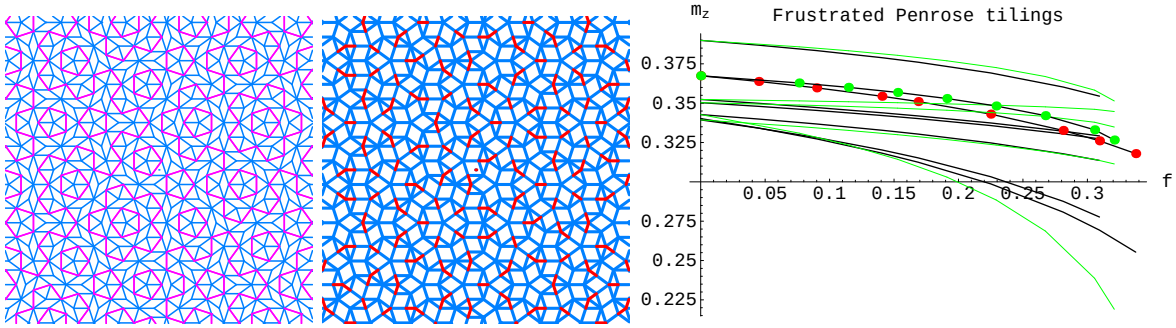

Figure 3. Frustrated Penrose tilings for case III (left) and case IV (middle) showing the J-bonds in blue and the J' bonds in red. (right)Plots of the staggered magnetization averaged over all sites (red points: case III, green: case IV) and of different subsets of sites as a function of f

The spin wave spectrum and eigenmodes are calculated by the same technique that was used for the unfrustrated problem (see [3], namely, via a real space numerical diagonalization of the linearized spin wave Hamiltonian. The theory breaks down for large enough J', as in the preceding examples. Although a detailed analysis is still in progress, some results for the local staggered magnetizations are indicated in Fig. 3. The figure shows data for a system of 1686 spins in each of the two cases. For cases III and IV, the globally averaged staggered magnetization is shown, in red (III) and green (IV), as a function of f. The remaining curves show the decay of the average sublattice magnetization within each family, for the two problems. In each case, it is observed that one particular subset of sites reacts the most strongly to the perturbation. These subsets are the previously-mentioned $z = 5$ (case III) and $z = 4$ sites (caseIV), and they are also the sites of maximal quantum fluctuations in the absence of frustration. In these two examples of frustrating the Penrose tiling, the frustration acts to weaken the Néel order in different ways locally, with the same global result for the staggered magnetization. It will be interesting to explore different ways to add frustration, that involve, for example the higher coordination number sites ($z = 6, 7$), to see the effect on the decay of collinear magnetic order.

4. Conclusions

In inhomogeneous systems, quantum fluctuations suppress the local staggered magnetizations on certains subsets of sites. Several examples are presented here of the role of frustration in suppressing the Néel order in such systems. While the details of the suppression mechanism probably depend on the specific lattice structure, the trend observed here indicates more efficient suppression when frustration is added on highly connected sites.

[1] Jagannathan A, Wessel S and Moessner R 2006 *Phys. Rev.* B **74** 184410
[2] The dependence of m_{si} on coordination number is not necessarily monotonic, since next nearest neighbor effects are also relevant.
[3] Szallas A, Jagannathan A, Wessel S and Duneau M 2007 *Phys. Rev.* B **75** 212407; Szallas A and Jagannathan A 2008 *Phys. Rev.* B **77** 104427